INFRARED PROBLEM FOR THE NELSON MODEL ON STATIC SPACE-TIMES

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Abstract. We consider the Nelson model on some static space-times and investigate the problem of existence of a ground state. Nelson models with variable coefficients arise when one replaces in the usual Nelson model the flat Minkowski metric by a static metric, allowing also the boson mass to depend on position. We investigate the existence of a ground state of the Hamiltonian in the presence of the infrared problem, i.e. assuming that the boson mass $m(x)$ tends to 0 at spatial infinity. We show that if $m(x) \geq C|x|^{-1}$ at infinity for some $C > 0$ then the Nelson Hamiltonian has a ground state.

1. Introduction

The study of Quantum Field Theory on curved space-times has seen important developments since the seventies. Probably the most spectacular prediction in this domain is the *Hawking effect* [Ha, FH, Ba], predicting that a star collapsing to a black hole asymptotically emits a thermal radiation. A related effect is the *Unruh effect* [Un, Un-W, dB-M], where an accelerating observer in Minkowski space-time sees the vacuum state as a thermal state.

Another important development is the use of *microlocal analysis* to study free or quasi-free states on globally hyperbolic space-times, which started with the seminal work by Radzikowski [Ra1, Ra2] , who proved that Hadamard states (the natural substitutes for vacuum states on curved space-times) can be characterized in terms of microlocal properties of their two-point functions. The use of microlocal analysis in this domain was further developed for example in [BFK], [Sa].

Most of these works deal with free or quasi-free states, because of the well-known difficulty to construct an interacting, relativistic quantum field theory, even on Minkowski space-time.

However in recent years a lot of effort was devoted to the rigorous study of *interacting* non-relativistic models on Minkowski space-time, typically obtained by coupling a relativistic quantum field to non-relativistic particles. The two main examples are *non-relativistic QED*, where the quantized Maxwell field is minimally coupled to a non-relativistic particle and the *Nelson model*, where a scalar bosonic field is linearly coupled to a non-relativistic particle. For both models it is necessary to add an ultraviolet cutoff in the interaction term to rigorously construct the associated Hamiltonian.

In both cases the models can be constructed on a Fock space with relatively little efforts, and several properties of the quantum Hamiltonian H can be rigorously studied. One of them, which will also be our main interest in this paper, is the question of the *existence of a ground state*. Obviously the fact that H has a ground state is an important physical property of the Nelson model. For example a consequence of the existence of a ground state is that *scattering states* can quite

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easily be constructed. These states describe the ground state of H with a finite number of additional asymptotically free bosons.

When H has no ground state one usually speaks of the *infrared problem* or *infrared divergence*. The infrared problem arises when the emission probability of bosons becomes infinite with increasing wave length. If the infrared problem occurs, the scattering theory has to be modified: all scattering states contain an infinite number of low energy (soft) bosons (see eg [DG3]). Among many papers devoted to this question, let us mention [AHH, BFS, BHLMS, G, H, LMS, Sp] for the Nelson model, and [GLL] for non-relativistic QED.

Our goal in this paper is to study the existence of a ground state for the Nelson model on a *static* space-time, allowing also for a position-dependent mass. This model is obtained by linearly coupling the Lagrangians of a Klein-Gordon field and of a non-relativistic particle on a static space-time (see Subsect. 2.2). We believe that this model, although non-relativistic, is an interesting testing ground for the generalization of results for free or quasi-free models on curved space-times to some interacting situations. Let us also mention that for the Nelson model on Minkowski space-time the removal of the ultraviolet cutoff can be done by relatively easy arguments. After removal of the ultraviolet cutoff, the Nelson model becomes a *local* (although non-relativistic) QFT model. In a subsequent paper [GHPS3], we will show that the ultraviolet cutoff can be removed for the Nelson model on a static space-time.

Most of our discussion will be focused on the role of the variable mass term on the ground state existence. Note that when one considers a massive Klein-Gordon field in the Schwarzschild metric, the effective mass tends to 0 at the black hole horizon (see eg [Ba]). We believe that the study of the Nelson model with a variable mass vanishing at spatial infinity will be a first step towards the extension of the rigorous justification of the Hawking effect in [Ba] to some interacting models.

1.1. **The Nelson model on Minkowski space-time.** In this subsection we quickly describe the usual Nelson model on Minkowski space-time. The *Nelson* model describes a scalar bosonic field linearly coupled to a quantum mechanical particle. It is formally defined by the Hamiltonian

$$H = \frac{1}{2}p^2 + W(q) + \frac{1}{2}\int_{\mathbb{R}^3} \pi^2(\mathrm{x}) + (\nabla\varphi(\mathrm{x}))^2 + m^2\varphi^2(\mathrm{x})\mathrm{dx} + \int_{\mathbb{R}^3} \varphi(\mathrm{x})\rho(\mathrm{x}-q)\mathrm{dx},$$

where ρ denotes a cutoff function, p, q denote the position and momentum of the particle, $W(q)$ is an external potential and $\varphi(\mathrm{x})$, $\pi(\mathrm{x})$ are the canonical field position and momentum.

The Nelson model arises from the quantization of the following coupled Klein-Gordon and Newton system:

$$\left\{\begin{array}{l} (\Box + m^2)\varphi(t,\mathrm{x}) = -\rho(\mathrm{x}-q_t), \\ \ddot{q}_t = -\nabla_q W(q_t) - \int \varphi(t,\mathrm{x})\nabla_{\mathrm{x}}\rho(\mathrm{x}-q_t)\mathrm{dx}, \end{array}\right. \tag{1.1}$$

were $\Box$ denotes the d'Alembertian on the Minkowski space-time $\mathbb{R}^{1+3}$. The cutoff function ρ plays the role of an ultraviolet cutoff and amounts to replacing the quantum mechanical point particle by a charge density.

To distinguish the Nelson model on Minkowski space-time from its generalizations that will be described later in the introduction, we will call it the *usual* (or *constant coefficients*) *Nelson model*.

For the usual Nelson model the situation is as follows: one assumes a stability condition (see Subsect. 4.5), implying that states with energy close to the bottom of the spectrum are localized in the particle position. Then if the bosons are massive

i.e. if $m > 0$ H has a ground state (see eg [G]). On the contrary if $m = 0$ and $\int \rho(x)\mathrm{d}x \neq 0$ then H has no ground state (see [DG3]).

1.2. **The Nelson model with variable coefficients.** We now describe a generalization of the usual Nelson model, obtained by replacing the free Laplacian $-\Delta_{\mathrm{x}}$ by a general second order differential operator and the constant mass term m by a function $m(\mathrm{x})$. We set:

$$h := -\sum_{1\leq j,k\leq d} c(\mathrm{x})^{-1}\partial_j a^{jk}(\mathrm{x})\partial_k c(\mathrm{x})^{-1} + m^2(\mathrm{x}),$$

for a Riemannian metric $a_{jk}\mathrm{dx}^j\mathrm{dx}^k$ and two functions $c(\mathrm{x})$, $m(\mathrm{x}) > 0$, and consider the generalization of (1.1):

$$\left\{\begin{array}{l} \partial_t^2\phi(t,\mathrm{x}) + h\phi(t,\mathrm{x}) + \rho(\mathrm{x}-q_t) = 0, \\ \ddot{q}_t = -\nabla_{\mathrm{x}}W(q_t) - \int_{\mathbb{R}^3}\phi(t,\mathrm{x})\nabla_{\mathrm{x}}\rho(\mathrm{x}-q_t)|g|^{\frac{1}{2}}\mathrm{d}^3\mathrm{x}. \end{array}\right. \tag{1.2}$$

Quantizing the field equations (1.2), we obtain a Hamiltonian H acting on the Hilbert space $L^2(\mathbb{R}^3)\otimes\Gamma_{\mathrm{s}}(L^2(\mathbb{R}^3))$ (see Sect. 3), which we call a *Nelson Hamiltonian with variable coefficients*. Formally H is defined by the following expression:

(1.3)

$$\begin{aligned} H =& \frac{1}{2}p^2 + W(q) \\ &+\frac{1}{2}\int_{\mathbb{R}^3}\pi^2(\mathrm{x}) + \sum_{jk}\partial_j\big(c(\mathrm{x})^{-1}\varphi(\mathrm{x})\big)a^{jk}(\mathrm{x})\big(\partial_k c(\mathrm{x})^{-1}\varphi(\mathrm{x})\big) + m^2(\mathrm{x})\varphi^2(\mathrm{x})\mathrm{dx} \\ &+\int_{\mathbb{R}^3}\varphi(\mathrm{x})\rho(\mathrm{x}-q)\mathrm{dx}. \end{aligned}$$

The main example of a variable coefficients Nelson model is obtained by replacing in the usual Nelson model the flat Minkowski metric on $\mathbb{R}^{1+3}$ by a *static* Lorentzian metric, and by allowing also the mass m to be position dependent. Recall that a static metric on $\mathbb{R}^{1+3}$ is of the form

$$g_{\mu\nu}(x)\mathrm{d}x^\mu\mathrm{d}x^\nu = -\lambda(\mathrm{x})\mathrm{d}t\mathrm{d}t + \lambda(x)^{-1}h_{\alpha\beta}(\mathrm{x})\mathrm{dx}^\alpha\mathrm{dx}^\beta,$$

where $x = (t,\mathrm{x}) \in \mathbb{R}^{1+3}$, $\lambda(\mathrm{x}) > 0$ is a smooth function, and $h_{\alpha,\beta}(\mathrm{x})$ is a Riemannian metric on $\mathbb{R}^3$. We show in Subsect. 2.3 that the natural Lagrangian for a point particle coupled to a scalar field on $(\mathbb{R}^{1+3}, g)$ leads (after a change of field variables) to the system (1.2).

1.3. **The infrared problem.** Assuming reasonable hypotheses on the matrix $[a^{jk}](\mathrm{x})$ and the functions $c(\mathrm{x})$, $m(\mathrm{x})$ it is easy to see that the formal expression (1.3) can be rigorously defined as a bounded below selfadjoint operator H.

The question we address in this paper is the problem of existence of a ground state for H. Variable coefficients Nelson models are examples of an abstract class of QFT Hamiltonians called *abstract Pauli-Fierz Hamiltonians* (see eg [G], [BD] and Subsect. 4.1). If ω is the *one-particle energy*, the constant $m := \inf\sigma(\omega)$ can be called the (rest) mass of the bosonic field, and abstract Pauli-Fierz Hamiltonians fall naturally into two classes: massive models if $m > 0$ and massless if $m = 0$.

For massive models, H typically has a ground state, if we assume either that the quantum particle is confined or a stability condition (see Subsect. 4.5). In this paper we concentrate on the massless case and hence our typical assumption will be that

$$\lim_{\mathrm{x}\to\infty} m(\mathrm{x}) = 0.$$

It follows that bosons of arbitrarily small energy may be present. The main result of this paper is that the existence or non-existence of a ground state for H depends on the rate of decay of the function $m(\mathrm{x})$. In fact we show in Thm. 4.1 that if

$$m(\mathrm{x}) \geq a\langle \mathrm{x}\rangle^{-1}, \text{ for some } a > 0,$$

and if the quantum particle is confined, then H has a ground state. In a subsequent paper [GHPS2], we will show that if

$$0 \leq m(\mathrm{x}) \leq C\langle \mathrm{x}\rangle^{-1-\epsilon}, \text{ for some } \epsilon > 0,$$

then H has no ground state. Therefore Thm. 4.1 is sharp with respect to the decay rate of the mass at infinity.

(If $h = -\Delta + \lambda m^2(\mathrm{x})$ for $m(\mathrm{x}) \in O(\langle \mathrm{x}\rangle^{-3/2})$ and the coupling constant λ is sufficiently small the same result is shown in [GHPS1]).

1.4. Notation.

We collect here some notation for the reader's convenience.

If $x \in \mathbb{R}^d$, we set $\langle x\rangle = (1+x^2)^{\frac{1}{2}}$.

The domain of a linear operator A on some Hilbert space $\mathcal{H}$ will be denoted by $\mathrm{Dom}A$, and its spectrum by $\sigma(A)$.

If $\mathfrak{h}$ is a Hilbert space, the *bosonic Fock space* over $\mathfrak{h}$ denoted by $\Gamma_{\mathrm{s}}(\mathfrak{h})$ is

$$\Gamma_{\mathrm{s}}(\mathfrak{h}) := \bigoplus_{n=0}^{\infty} \otimes_{\mathrm{s}}^n \mathfrak{h}.$$

We denote by $a^*(h)$, $a(h)$ for $h \in \mathfrak{h}$ the *creation/annihilation operators* acting on $\Gamma_{\mathrm{s}}(\mathfrak{h})$. The (Segal) *field operators* $\phi(h)$ are defined as $\phi(h) := \frac{1}{\sqrt{2}}(a^*(h) + a(h))$.

If $\mathcal{K}$ is another Hilbert space and $v \in B(\mathcal{K}, \mathcal{K}\otimes\mathfrak{h})$, then one defines the operators $a^*(v)$, $a(v)$ as unbounded operators on $\mathcal{K}\otimes\Gamma_{\mathrm{s}}(\mathfrak{h})$ by:

$$\begin{aligned}
&a^*(v)\Big|_{\mathcal{K}\otimes\bigotimes_{\mathrm{s}}^n \mathfrak{h}} := \sqrt{n+1}\Big(\mathbb{1}_{\mathcal{K}}\otimes\mathcal{S}_{n+1}\Big)\Big(v\otimes\mathbb{1}_{\bigotimes_{\mathrm{s}}^n \mathfrak{h}}\Big),\\
&a(v) := \big(a^*(v)\big)^*,\\
&\phi(v) := \tfrac{1}{\sqrt{2}}(a(v) + a^*(v)).
\end{aligned}$$

They satisfy the estimates

$$\|a^\sharp(v)(N+1)^{-\frac{1}{2}}\| \leq \|v\|, \tag{1.4}$$

where $\|v\|$ is the norm of v in $B(\mathcal{K}, \mathcal{K}\otimes\mathfrak{h})$.

If b is a selfadjoint operator on $\mathfrak{h}$ its second quantization $\mathrm{d}\Gamma(b)$ is defined as:

$$d\Gamma(b)\Big|_{\bigotimes_{\mathrm{s}}^n \mathfrak{h}} := \sum_{j=1}^{n} \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{j-1}\otimes b\otimes\underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{n-j}.$$

2. The Nelson model on static space-times

In this section we discuss the Nelson model on static space-times, which is the main example of Hamiltonians that will be studied in the rest of the paper. It is convenient to start with the Lagrangian framework.

2.1. Klein-Gordon equation on static space-times.

Let $g_{\mu\nu}(x)$ be a Lorentzian metric of signature $(-,+,+,+)$ on $\mathbb{R}^{1+3}$. Set $|g| = \det[g_{\mu\nu}]$, $[g^{\mu\nu}] = [g_{\mu\nu}]^{-1}$. Consider the Lagrangian

$$L_{\mathrm{free}}(\phi)(x) = \frac{1}{2}\partial_\mu\phi(x)g^{\mu\nu}(x)\partial_\nu\phi(x) + \frac{1}{2}m^2(x)\phi^2(x),$$

for a function $m : \mathbb{R}^4 \to \mathbb{R}^+$ and the associated action:

$$S_{\mathrm{field}}(\phi) = \int_{\mathbb{R}^4} L_{\mathrm{free}}(\phi)(x)|g|^{\frac{1}{2}}(x)\mathrm{d}^4x,$$

where $\phi : \mathbb{R}^4 \to \mathbb{R}$. The Euler-Lagrange equations yield the *Klein-Gordon equation*:

$$\Box_g \phi + m^2(x)\phi = 0,$$

for

$$\Box_g = -|g|^{-\frac{1}{2}}\partial_\mu |g|^{\frac{1}{2}} g^{\mu\nu}\partial_\nu.$$

Usually one has

$$\frac{1}{2}m^2(x) = \frac{1}{2}(m^2 + \theta R(x)),$$

where $m \geq 0$ is the mass and $R(x)$ is the scalar curvature of the metric $g_{\mu\nu}$, (assuming of course that the function on the right is positive). In particular if $m = 0$ and $\theta = \frac{1}{6}$ one obtains the so-called conformal wave equation.

We set $x = (t, \mathrm{x}) \in \mathbb{R}^{1+3}$. The metric $g_{\mu\nu}$ is *static* if:

$$g_{\mu\nu}(x)\mathrm{d}x^\mu \mathrm{d}x^\nu = -\lambda(\mathrm{x})\mathrm{d}t\mathrm{d}t + \lambda(x)^{-1} h_{\alpha\beta}(\mathrm{x})\mathrm{d}\mathrm{x}^\alpha \mathrm{d}\mathrm{x}^\beta,$$

where $\lambda(\mathrm{x}) > 0$ is a smooth function and $h_{\alpha\beta}$ is a Riemannian metric on $\mathbb{R}^3$. We assume also that $m^2(x) = m^2(\mathrm{x})$ is independent on t.

Setting $\phi(t, \mathrm{x}) = \lambda |h|^{-1/4}\tilde{\phi}(t, \mathrm{x})$, we obtain that $\tilde{\phi}(t, \mathrm{x})$ satisfies the equation:

$$\partial_t^2 \tilde{\phi} - \lambda |h|^{-1/4}\partial_\alpha |h|^{\frac{1}{2}} h^{\alpha\beta}\partial_\beta |h|^{-1/4}\lambda\tilde{\phi} + m^2\lambda\tilde{\phi} = 0.$$

We note that $|h|^{-1/4}\partial_\alpha |h|^{\frac{1}{2}} h^{\alpha\beta}\partial_\beta |h|^{-1/4}$ is (formally) self-adjoint on $L^2(\mathbb{R}^3, \mathrm{dx})$ and is the Laplace-Beltrami operator $\Delta_h$associated to the Riemannian metric $h_{\alpha\beta}$ (after the usual density change $u \mapsto |h|^{1/4}u$ to work on the Hilbert space $L^2(\mathbb{R}^3, \mathrm{dx})$).

2.2. **Klein-Gordon field coupled to a non-relativistic particle.** We now couple the Klein-Gordon field to a non-relativistic particle. We fix a mass $M > 0$, a charge density $\rho : \mathbb{R}^3 \to \mathbb{R}^+$ with $q = \int_{\mathbb{R}^3} \rho(\mathrm{y})\mathrm{d}^3\mathrm{y} \neq 0$ and a real potential $W : \mathbb{R}^3 \to \mathbb{R}$. The action for the coupled system is

$$S = S_{\mathrm{part}} + S_{\mathrm{field}} + S_{\mathrm{int}},$$

for

$$\begin{aligned} S_{\mathrm{part}} &= \textstyle\int_{\mathbb{R}} \frac{M}{2}|\dot{\mathrm{x}}(t)|^2 - W(\mathrm{x}(t))\mathrm{d}t, \\ S_{\mathrm{int}} &= \textstyle\int_{\mathbb{R}^4} \phi(t, \mathrm{x})\rho(\mathrm{x} - \mathrm{x}(t))|g|^{\frac{1}{2}}(x)\mathrm{d}^4 x. \end{aligned}$$

The Euler-Lagrange equations are:

$$\begin{cases} \Box_g \phi(t, \mathrm{x}) + m^2(t, \mathrm{x})\phi(t, \mathrm{x}) + \rho(\mathrm{x} - \mathrm{x}(t)) = 0, \\ M\ddot{\mathrm{x}}(t) = -\nabla_{\mathrm{x}} W(\mathrm{x}(t)) - \int_{\mathbb{R}^3} \phi(t, \mathrm{x})\nabla_{\mathrm{x}}\rho(\mathrm{x} - \mathrm{x}(t))|g|^{\frac{1}{2}}\mathrm{d}^3\mathrm{x}. \end{cases}$$

Doing the same change of field variables as in Subsect. 2.1 and deleting the tildes, we obtain the system:

$$\begin{cases} \partial_t^2 \phi - \lambda\Delta_h \lambda\phi + m^2\lambda\phi + \rho(\mathrm{x} - \mathrm{x}(t)) = 0, \\ M\ddot{\mathrm{x}}(t) = -\nabla W(\mathrm{x}(t)) - \int_{\mathbb{R}^3} \phi(t, \mathrm{x})\nabla\rho(\mathrm{x} - \mathrm{x}(t))d^3\mathrm{x}. \end{cases} \tag{2.1}$$

2.3. **The Nelson model on a static space-time.** If the metric is static, the equations (2.1) are clearly Hamiltonian equations for the classical Hamiltonian $H = H_{\mathrm{part}} + H_{\mathrm{field}} + H_{\mathrm{int}}$, where:

$$H_{\mathrm{part}}(\mathrm{x}, \xi) = \frac{1}{2M}\xi^2 + W(\mathrm{x}),$$

$$\begin{aligned} &H_{\mathrm{field}}(\varphi, \pi) \\ = \;& \tfrac{1}{2}\textstyle\int_{\mathbb{R}^3} \pi^2(\mathrm{x}) - \varphi(\mathrm{x})\lambda(\mathrm{x})\Delta_h \lambda(\mathrm{x})\varphi(\mathrm{x}) + m^2(\mathrm{x})\lambda(\mathrm{x})\varphi^2(\mathrm{x})\mathrm{d}\mathrm{x}, \end{aligned}$$

$$H_{\mathrm{int}}(\mathrm{x}, \xi, \varphi, \pi) = \int_{\mathbb{R}^3} \rho(\mathrm{y} - \mathrm{x})\varphi(\mathrm{y})\mathrm{d}\mathrm{y}.$$

The classical phase space is as usual $\mathbb{R}^3 \times \mathbb{R}^3 \times L^2_{\mathbb{R}}(\mathbb{R}^3) \times L^2_{\mathbb{R}}(\mathbb{R}^3)$, with the symplectic form

$$(\mathrm{x}, \xi, \varphi, \pi)\omega(\mathrm{x}', \xi', \varphi', \pi') = \mathrm{x} \cdot \xi' - \mathrm{x}' \cdot \xi + \int_{\mathbb{R}^3} \varphi(\mathrm{x})\pi'(\mathrm{x}) - \pi(\mathrm{x})\varphi'(\mathrm{x})\mathrm{dx}.$$

The usual quantization scheme leads to the Hilbert space:

$$L^2(\mathbb{R}^3, \mathrm{dy}) \otimes \Gamma_{\mathrm{s}}(L^2(\mathbb{R}^3, \mathrm{dx})),$$

where $\Gamma_{\mathrm{s}}(\mathfrak{h})$ is the bosonic Fock space over the one-particle space $\mathfrak{h}$, and to the quantum Hamiltonian:

$$H = (-\frac{1}{2}\Delta_{\mathrm{y}} + W(\mathrm{y})) \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega) + \frac{1}{\sqrt{2}}\left(a^*(\omega^{-\frac{1}{2}}\rho(\cdot - \mathrm{y}) + a(\omega^{-\frac{1}{2}}\rho(\cdot - \mathrm{y})\right),$$

where

$$\omega = (-\lambda\Delta_h\lambda + m^2\lambda)^{\frac{1}{2}},$$

$\mathrm{d}\Gamma(\omega)$ is the usual second quantization of ω and $a^*(f)$, $a(f)$ are the creation/annihilation operators on $\Gamma_{\mathrm{s}}(L^2(\mathbb{R}^3, \mathrm{dx}))$.

3. The Nelson Hamiltonian with variable coefficients

In this section we define the Nelson model with variable coefficients that will be studied in the rest of the paper. We will deviate slightly from the notation in Sect. 2 by denoting by $x \in \mathbb{R}^3$ (resp. $X \in \mathbb{R}^3$) the boson (resp. electron) position. As usual we set $D_x = \mathrm{i}^{-1}\nabla_x$, $D_X = \mathrm{i}^{-1}\nabla_X$.

3.1. **Electron Hamiltonian.**

We define the electron Hamiltonian as:

$$K := K_0 + W(X),$$

where

$$K_0 = \sum_{1 \le j,k \le 3} D_{X_j} A^{jk}(X) D_{X_k},$$

acting on $\mathcal{K} := L^2(\mathbb{R}^3, \mathrm{d}X)$, where:

$$(E1) \;\; C_0\mathbb{1} \le [A^{jk}(X)] \le C_1\mathbb{1}, \; C_0 > 0.$$

We assume that $W(X)$ is a real potential such that $K_0 + W$ is essentially selfadjoint and bounded below. We denote by K the closure of $K_0 + W$. Later we will assume the following *confinement condition* :

$$(E2) \;\; W(X) \ge C_0\langle X\rangle^{2\delta} - C_1, \text{ for some } \delta > 0.$$

Physically this condition means that the electron is confined. As is well known (see eg [GLL]) for the question of existence of a ground state , this condition can be replaced by a *stability condition*, meaning that states near the bottom of the spectrum of the Hamiltonian are confined in the electronic variables by energy conservation.

We will discuss the extension of our results when one assume the stability condition in Subsect. 4.5.

3.2. **Field Hamiltonian.** Let:

$$\begin{aligned} h_0 :=& -\sum_{1\leq j,k\leq d} c(x)^{-1}\partial_j a^{jk}(x)\partial_k c(x)^{-1}, \\ h :=& \ h_0 + m^2(x), \end{aligned}$$

with a^{jk}, c, m are real functions and:

$$(B1) \quad \begin{array}{l} C_0 \mathbb{1} \leq [a^{jk}(x)] \leq C_1 \mathbb{1},\ C_0 \leq c(x) \leq C_1,\ C_0 > 0, \\ \partial_x^\alpha a^{jk}(x) \in O(\langle x\rangle^{-1}),\ |\alpha| \leq 1,\ \partial_x^\alpha c(x) \in O(1),\ |\alpha| \leq 2, \\ \partial_x^\alpha m(x) \in O(1),\ |\alpha| \leq 1. \end{array}$$

Clearly h is selfadjoint on $H^2(\mathbb{R}^3)$ and $h \geq 0$. The *one-particle space* and *one-particle energy* are:

$$\mathfrak{h} := L^2(\mathbb{R}^3, \mathrm{d}x),\ \omega := h^{\frac{1}{2}}.$$

The constant:

$$\inf \sigma(\omega) =: m \geq 0,$$

can be viewed as the *mass* of the scalar bosons.

The following lemma is easy;

Lemma 3.1. (1) *One has* $\mathrm{Ker}\omega = \{0\}$*,*
(2) *Assume in addition to (B1) that* $\lim_{x\to\infty} m(x) = 0$*. Then* $\inf \sigma(\omega) = 0$*.*

Proof. It follows from (B1) that

$$(u|hu) \leq C_1(c^{-1}u| - \Delta c^{-1}u) + (c^{-1}u|c^{-1}m^2u),\ u \in H^2(\mathbb{R}^3).$$

Therefore if $hu = 0$ u is constant. It follows also from (B1) that $c(x)^{-1}$ preserves $H^2(\mathbb{R}^3)$. Therefore by the variational principle

$$m^2 = \inf \sigma(h) \leq C_1 \inf \sigma(-\Delta + c^{-2}(x)m^2(x)) = 0.$$

This proves (2). □

The Nelson Hamiltonian defined below will be called *massive* (resp. *massless*) if $m > 0$ (resp. $m = 0$.) The field Hamiltonian is

$$\mathrm{d}\Gamma(\omega),$$

acting on the bosonic Fock space $\Gamma_{\mathrm{s}}(\mathfrak{h})$.

3.3. **Nelson Hamiltonian.** Let $\rho \in S(\mathbb{R}^3)$, with $\rho \geq 0$, $q = \int_{\mathbb{R}^3} \rho(y)\mathrm{d}y \neq 0$. We set:

$$\rho_X(x) = \rho(x - X)$$

and define the *UV cutoff fields* as:

$$\varphi_\rho(X) := \phi(\omega^{-\frac{1}{2}}\rho_X), \tag{3.1}$$

where for $f \in \mathfrak{h}$, $\phi(f)$ is the Segal field operator:

$$\phi(f) := \frac{1}{\sqrt{2}}\left(a^*(f) + a(f)\right).$$

Note that setting

$$\varphi(X) := \phi(\omega^{-\frac{1}{2}}\delta_X),$$

one has $\varphi_\rho(X) = \int \varphi(X - Y)\rho(Y)\mathrm{d}Y$.

Remark 3.2. *One can think of another definition of UV cutoff fields, namely:*

$$\tilde{\varphi}_\chi(X) := \phi(\omega^{-\frac{1}{2}}\chi(\omega)\delta_X),$$

for $\chi \in S(\mathbb{R})$, $\chi(0) = 1$*. In the constant coefficients case where* $h = -\Delta$ *both definitions are equivalent. In the variable coefficients case the natural definition (3.1) is much more convenient.*

The *Nelson Hamiltonian* is:

$$H := K \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega) + \varphi_\rho(X), \tag{3.2}$$

acting on

$$\mathcal{H} = \mathcal{K} \otimes \Gamma_{\mathrm{s}}(\mathfrak{h}).$$

Set also:

$$H_0 := K \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega),$$

which is selfadjoint on its natural domain. The following lemma is standard.

Lemma 3.3. *Assume hypotheses (E1), (B1). Then H is selfadjoint and bounded below on $D(H_0)$.*

Proof. it suffices to apply results on abstract Pauli-Fierz Hamiltonians (see eg [GGM, Sect.4]). H is an abstract Pauli-Fierz Hamiltonian with coupling operator $v \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$ equal to:

$$L^2(\mathbb{R}^3, \mathrm{d}X) \ni u \mapsto \omega^{-\frac{1}{2}} \rho(x - X) u(X) \in L^2(\mathbb{R}^3, \mathrm{d}X) \otimes L^2(\mathbb{R}^3, \mathrm{d}x)$$

Applying [GGM, Corr. 4.4], it suffices to check that $\omega^{-\frac{1}{2}} v \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$. Now

$$\|\omega^{-\frac{1}{2}} v\|_{B(\mathcal{K}, \mathcal{K}\otimes\mathfrak{h})} = (\sup_{X \in \mathbb{R}^3} \|\omega^{-1} \rho_X\|^2)^{\frac{1}{2}}$$

Using that $h \geq C D_x^2$ and the Kato-Heinz inequality, we obtain that $\omega^{-2} \leq C|D_x|^{-2}$, hence it suffices to check that the map

$$L^2(\mathbb{R}^3, \mathrm{d}X) \ni u \mapsto |D_x|^{-1} \rho(x - X) u(X) \in L^2(\mathbb{R}^3, \mathrm{d}X) \otimes L^2(\mathbb{R}^3, \mathrm{d}x)$$

is bounded, which is well known. □

4. Existence of a ground state

In this section we will prove our main result about the existence of a ground state for variable coefficients Nelson Hamiltonians. This result will be deduced from an abstract existence result extending the one in [BD], whose proof is outlined in Subsects. 4.1, 4.2 and 4.3.

Theorem 4.1. *Assume hypotheses (E1), (B1). Assume in addition that:*

$$m(x) \geq a\langle x\rangle^{-1}, \ \textit{for some } a > 0,$$

and (E2) for some $\delta > \frac{3}{2}$. Then $\inf \sigma(H)$ is an eigenvalue.

Remark 4.2. *The condition $\delta > \frac{3}{2}$ in Thm. 4.1 comes from the operator bound $\omega^{-3} \leq C\langle x\rangle^{3+\epsilon}$, $\forall\, \epsilon > 0$ proved in Thm. A.8.*

Remark 4.3. *From Lemma 3.1 we know that $\inf \sigma(\omega) = 0$ if $\lim_{x\to\infty} m(x) = 0$. Therefore the Nelson Hamiltonian can be massless using the terminology of Subsect. 3.2.*

Remark 4.4. *In a subsequent paper* [GHPS2] *we will show that if*

$$0 \leq m(x) \leq C\langle x\rangle^{-1-\epsilon}, \ \textit{for some } \epsilon > 0,$$

then H has no ground state. Therefore the result of Thm. 4.1 is sharp with respect to the decay rate of the mass at infinity.

4.1. **Abstract Pauli-Fierz Hamiltonians.** In [BD], Bruneau and Dereziński study the spectral theory of abstract Pauli-Fierz Hamiltonians of the form

$$H = K \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega) + \phi(v),$$

acting on the Hilbert space $\mathcal{H} = \mathcal{K} \otimes \Gamma_{\rm s}(\mathfrak{h})$, where $\mathcal{K}$ is the Hilbert space for the small system and $\mathfrak{h}$ the one-particle space for the bosonic field. The Hamiltonian H is called massive (resp. massless) if $\inf \sigma(\omega) > 0$ (resp. $\inf \sigma(\omega) = 0$). Among other results they prove the existence of a ground state for H if v is infrared regular.

Although most of their hypotheses are natural and essentially optimal, we cannot directly apply their abstract results to our situation. In fact they assume (see [BD, Assumption E]) that the one-particle space $\mathfrak{h}$ equals $L^2(\mathbb{R}^d, \mathrm{d}k)$ and the one-particle energy ω is the multiplication operator by a function $\omega(k)$ which is positive, with $\nabla\omega$ bounded, and $\lim_{k\to\infty} \omega(k) = +\infty$. This assumption on the one-particle energy is only needed to prove an HVZ theorem for massive (or massless with an infrared cutoff) Pauli-Fierz Hamiltonians.

In our case this assumption could be deduced (modulo unitary equivalence) from the spectral theory of h. For example it would suffices to know that h is unitarily equivalent to $-\Delta$. This last property would follow from the absence of eigenvalues for h and from the scattering theory for the pair $(h, -\Delta)$ and require additional decay properties of the $[a^{ij}](x)$, $m(x)$ and of some of their derivatives.

We will replace it by more geometric assumptions on ω (see hypothesis (4.4) below), similar to those introduce in [GP], where abstract bosonic QFT Hamiltonians were considered. Since we do not aim for generality, our hypotheses on the coupling operator v are stronger than necessary, but lead to simpler proofs. Also most of the proofs will be only sketched.

Let $\mathfrak{h}, \mathcal{K}$ two Hilbert spaces and set $\mathcal{H} = \mathcal{K} \otimes \Gamma_{\rm s}(\mathfrak{h})$.

We fix selfadjoint operators $K \geq 0$ on $\mathcal{K}$ and $\omega \geq 0$ on $\mathfrak{h}$. We set

$$\inf \sigma(\omega) =: m \geq 0.$$

If $m = 0$ one has to assume additionally that $\mathrm{Ker}\omega = \{0\}$ (see Remark 4.5 for some explanation of this fact).

Remark 4.5. *It $\mathcal{X}$ is a real Hilbert space and ω is a selfadjoint operator on $\mathcal{X}$, the condition* $\mathrm{Ker}\omega = \{0\}$ *is well known to be necessary to have a stable quantization of the abstract Klein-Gordon equation $\partial_t^2\phi(t) + \omega^2\phi(t) = 0$ where $\phi(t) : \mathbb{R} \to \mathcal{X}$.*

If $\mathrm{Ker}\omega \neq \{0\}$ *the phase space $\mathcal{Y} = \mathcal{X} \oplus \mathcal{X}$ for the Klein-Gordon equation splits into the symplectic direct sum $\mathcal{Y}_{\rm reg} \oplus \mathcal{Y}_{\rm sing}$, for $\mathcal{Y}_{\rm reg} =$* $\mathrm{Ker}\omega^\perp \oplus \mathrm{Ker}\omega^\perp$, $\mathcal{Y}_{\rm sing} = \mathrm{Ker}\omega \oplus \mathrm{Ker}\omega$, *both symplectic spaces being invariant under the symplectic evolution associated to the Klein-Gordon equation. On $\mathcal{Y}_{\rm reg}$ one can perform the stable quantization. On $\mathcal{Y}_{\rm sing}$,if for example* $\mathrm{Ker}\omega$ *is $d-$dimensional, the quantization leads to the Hamiltonian $-\Delta$ on $L^2(\mathbb{R}^d)$. Clearly any perturbation of the form $\phi(f)$ for $\mathbb{1}_{\{0\}}(\omega)f \neq 0$ will make the Hamiltonian unbounded from below.*

So we will always assume that

$$\omega \geq 0,\ \mathrm{Ker}\omega = \{0\}. \tag{4.1}$$

Let $H_0 = \mathcal{K} \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega)$. We fix also a coupling operator v such that:

$$v \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h}). \tag{4.2}$$

The quadratic form $\phi(v) = a(v) + a^*(v)$ is well defined for example on $\mathcal{K} \otimes \mathrm{Dom} N^{\frac{1}{2}}$. We will also assume that:

$$\omega^{-\frac{1}{2}} v (K+1)^{-\frac{1}{2}} \text{ is compact.} \tag{4.3}$$

Proposition 4.6 ([BD] Thm. 2.2)**.** *Assume (4.1), (4.3). Then $H = H_0 + \phi(v)$ is well defined as a form sum and yields a bounded below selfadjoint operator with* $\mathrm{Dom}|H|^{\frac{1}{2}} = \mathrm{Dom}|H_0|^{\frac{1}{2}}$.

The operator H defined as above is called an abstract Pauli-Fierz Hamiltonian.

4.2. **Existence of a ground state for cutoff Hamiltonians.** We introduce as in [BD] the infrared-cutoff objects

$$v_\sigma = F(\omega \geq \sigma)v,\ H_\sigma = K \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega) + \phi(v_\sigma),\ \sigma > 0,$$

where $F(\lambda \geq \sigma)$ denotes as usual a function of the form $\chi(\sigma^{-1}\lambda)$, where $\chi \in C^\infty(\mathbb{R})$, $\chi(\lambda) \equiv 0$ for $\lambda \leq 1$, $\chi(\lambda) \equiv 1$ for $\lambda \geq 2$.

An important step to prove that H has a ground state is to prove that H_σ has a ground state. The usual trick is to consider

$$\tilde{H}_\sigma = K \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega_\sigma) + \phi(v_\sigma),$$

where:

$$\omega_\sigma := F(\omega \leq \sigma)\sigma + (1 - F(\omega \leq \sigma))\omega = \omega + (\sigma - \omega)F(\omega \leq \sigma).$$

Note that since $\omega_\sigma \geq \sigma > 0$, $\tilde{H}_\sigma$ is a massive Pauli-Fierz Hamiltonian. Moreover it is well known (see eg [G], [BD]) H_σ has a ground state iff $\tilde{H}_\sigma$ does. The fact that $\tilde{H}_\sigma$ has a ground state follows from an estimate on its essential spectrum (HVZ theorem). In [BD] this is shown using the condition that $\mathfrak{h} = L^2(\mathbb{R}^d, \mathrm{d}k)$ and $\omega = \omega(k)$. Here we will replace this condition by the following more abstract condition, formulated using an additional selfadjoint operator $\mathbf{r}$ on $\mathfrak{h}$. Similar abstract conditions were introduced in [GP].

We will assume that there exists an selfadjoint operator $\mathbf{r} \geq 1$ on $\mathfrak{h}$ such that the following conditions hold for all $\sigma > 0$:

$$\begin{aligned} &(i)\ (z - \mathbf{r})^{-1} :\ \mathrm{Dom}\omega_\sigma \to \mathrm{Dom}\omega_\sigma,\ \forall\ z \in \mathbb{C}\backslash\mathbb{R}, \\ &(ii)\ [\mathbf{r}, \omega_\sigma] \text{ defined as a quadratic form on } \mathrm{Dom}\mathbf{r} \cap \mathrm{Dom}\omega \text{ is bounded,} \\ &(iii)\ \mathbf{r}^{-\epsilon}(\omega_\sigma + 1)^{-\epsilon} \text{ is compact on } \mathfrak{h} \text{ for some } 0 < \epsilon < \tfrac{1}{2}. \end{aligned} \tag{4.4}$$

The operator $\mathbf{r}$, called a *gauge*, is used to localize particles in $\mathfrak{h}$.

We assume also as in [BD]:

$$(K + 1)^{-\frac{1}{2}} \text{ is compact.} \tag{4.5}$$

This assumption means that the small system is confined.

Proposition 4.7. *Assume (4.1), (4.2), (4.3), (4.4),(4.5) . Then*

$$\sigma_{\mathrm{ess}}(\tilde{H}_\sigma) \subset [\inf \sigma(\tilde{H}_\sigma) + \sigma, +\infty[.$$

It follows that $\tilde{H}_\sigma$ (and hence H_σ) has a ground state for all $\sigma > 0$.

Proof. By (4.3), $\phi(v_\sigma)$ is form bounded with respect to H_0 (and to $K \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\omega_\sigma)$) with the infinitesimal bound, hence H_σ, $\tilde{H}_\sigma$ are well defined as bounded below selfadjoint Hamiltonians.

We can follow the proof of [DG2, Thm. 4.1] or [GP, Thm. 7.1] for its abstract version. For ease of notation we denote simply $\tilde{H}_\sigma$ by H, ω_σ by ω and v_σ by v. The key estimate is the fact that for $\chi \in C_0^\infty(\mathbb{R})$ one has

$$\chi(H^{\mathrm{ext}})I^*(j^R) - I^*(j^R)\chi(H) \in o(1),\ \text{when } R \to \infty. \tag{4.6}$$

(The extended operator $H^{\rm ext}$ and identification operator $I(j^R)$ are defined for example in [GP, Sect.2.4]). The two main ingredients of the proof of (4.6) are the estimates:

$$[F(\frac{\mathbf{r}}{R}),\omega_\sigma]\in O(R^{-1}),\ F\in C_0^\infty(\mathbb{R}), \tag{4.7}$$

and

$$\omega_\sigma^{-\frac12}F(\frac{\mathbf{r}}{R}\geq 1)v_\sigma(K+1)^{-\frac12}\in o(R^0). \tag{4.8}$$

Now (4.8) follows from the fact that $v_\sigma(K+1)^{-\frac12}$ is compact (note that $\omega_\sigma^{-\frac12}$ is bounded since $\omega_\sigma\geq\sigma$), and (4.7) follows from Lemma 4.8. The estimate (4.6) can then be proved exactly as in [GP, Lemma 6.3]. Note that here we prove only the $\subset$ part of the HVZ theorem, which is sufficient for our purposes. The details are left to the reader. □

Lemma 4.8. *Assume conditions (i), (ii) of (4.4). Then for all $F\in C_0^\infty(\mathbb{R})$ one has:*

$$F(\mathbf{r}):\ {\rm Dom}\omega_\sigma\to{\rm Dom}\omega_\sigma,$$
$$[F(\tfrac{\mathbf{r}}{R}),\omega_\sigma]\in O(R^{-1}).$$

Proof. The proof of the lemma is easy, using almost analytic extensions, as for example in [GP]. The details are left to the interested reader. □

4.3. **Existence of a ground state for massless models.** Let us introduce the following hypothesis on the coupling operator ([BD, Hyp. F]):

$$\omega^{-1}v(K+1)^{-\frac12}\text{ is compact.} \tag{4.9}$$

Theorem 4.9. *Assume (4.1), (4.2), (4.3), (4.4), (4.5) and (4.9). Then H has a ground state.*

Proof. we can follow the proof in [BD, Sect. 4]. The existence of ground state for H_σ ([BD, Prop. 4.5]) is shown in Prop. 4.7. The arguments in [BD, Sects 4.2, 4.3] based on the pull-through and double pull-through formulas are abstract and valid for any one particle operator ω. The only place where the fact that $\mathfrak{h}=L^2(\mathbb{R}^d,{\rm d}k)$ and $\omega=\omega(k)$ appears is in [BD, Prop. 4.7] where the operator $|x|=|{\rm i}\nabla_k|$ enters. In our situation it suffices to replace it by our gauge operator $\mathbf{r}$. The rest of the proof is unchanged. □

4.4. **Proof of Thm. 4.1.** We now complete the proof of Thm. 4.1, by verifying the hypotheses of Thm. 4.9. We recall that $\mathfrak{h}=L^2(\mathbb{R}^d{\rm d}x)$, $\omega=h^{\frac12}$ and we will take $\mathbf{r}=\langle x\rangle=(1+x^2)^{\frac12}$.

Proof of Thm. 4.1.

We saw in the proof of Lemma 3.3 that $v,\omega^{-\frac12}v$ are bounded, hence in particular (4.2) is satisfied. By hypothesis (E2), $(K+1)^{-\frac12}$ is compact, which implies that conditions (4.3) and (4.5) are satisfied.

We now check condition (4.4). Note that $\omega_\sigma=f(h)$ where $f\in C^\infty(\mathbb{R})$ with $f(\lambda)=\lambda^{\frac12}$ for $\lambda\geq 2$. Clearly ${\rm Dom}\omega_\sigma=H^1(\mathbb{R}^d)$ which is preserved by $(z-\langle x\rangle)^{-1}$, so (i) of (4.4) is satisfied. Condition (iii) is also obviously satisfied. It remains to check condition (ii). To this end we write $\omega_\sigma=f(h)=(h+1)g(h)$ where $g\in C^\infty(\mathbb{R})$ satisfies

$$g^{(n)}(\lambda)\in O(\langle\lambda\rangle^{-\frac12-n}),\ n\in\mathbb{N},$$

and hence

$$[\langle x\rangle,\omega_\sigma]=[\langle x\rangle,h]g(h)+(h+1)[\langle x\rangle,g(h)]. \tag{4.10}$$

Since $\nabla a^{jk}(x)$, $\nabla c(x)$, $\nabla m(x)$ are bounded and $\mathrm{Dom} h = H^2(\mathbb{R}^d)$ we see that

$$[\langle x\rangle, h](h+1)^{-\frac{1}{2}}, [[\langle x\rangle, h], h](h+1)^{-1} \text{ are bounded.} \tag{4.11}$$

In particular the first term in the r.h.s. of (4.10) is bounded. To estimate the second term, we use an almost analytic extension of g satisfying:

$$\begin{array}{l}\tilde{g}_{|\mathbb{R}} = g,\ |\frac{\partial \tilde{g}}{\partial \bar{z}}(z)| \leq C_N \langle z\rangle^{-3/2-N}|\mathrm{Im} z|^N,\ N \in \mathbb{N},\\ \mathrm{supp}\tilde{g} \subset \{z \in \mathbb{C} | |\mathrm{Im} z| \leq c(1+|\mathrm{Re} z|)\},\end{array} \tag{4.12}$$

(see eg [DG1, Prop. C.2.2]), and write

$$g(h) = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial \tilde{g}}{\partial \bar{z}}(z)(z-h)^{-1}\mathrm{d}z \wedge \mathrm{d}\bar{z}.$$

We perform a commutator expansion to obtain that:

$$[\langle x\rangle, g(h)] = g'(h)[\langle x\rangle, h] + R_2,$$

for

$$R_2 = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial \tilde{g}}{\partial \bar{z}}(z)(z-h)^{-2}[[\langle x\rangle, h]h](z-h)^{-1}\mathrm{d}z \wedge \mathrm{d}\bar{z}.$$

Since $|g'(\lambda)| \leq C\langle\lambda\rangle^{-3/2}$, $(h+1)g'(h)[\langle x\rangle, h]$ is bounded. To estimate the term $(h+1)R_2$, we use again (4.11) and the bound

$$\|(h+1)^{\alpha}(z-h)^{-1}\| \leq C\langle z\rangle^{\alpha}|\mathrm{Im} z|^{-1},\ \alpha = \frac{1}{2}, 1.$$

We obtain that

$$\|(h+1)R_2\| \leq C\|[[\langle x\rangle, h]h](h+1)^{-1}\| \int_{\mathbb{C}} |\frac{\partial \tilde{g}}{\partial \bar{z}}(z)|\langle z\rangle^2|\mathrm{Im} z|^{-3}\mathrm{d}z\mathrm{d}\bar{z}.$$

This integral is convergent using the estimate (4.12). This completes the proof of (4.4).

It remains to check condition (4.9), i.e. the fact that the interaction is infrared regular. This is the only place where the lower bound on $m(x)$ enters. By Thm. A.8 we obtain that $\omega^{-3/2}\langle x\rangle^{-3/2-\epsilon}$ is bounded for all $\epsilon > 0$. By condition (E2), we obtain that $\langle X\rangle^{3/2+\epsilon}(K+1)^{-\frac{1}{2}}$ is bounded for all $\epsilon > 0$ small enough.

Therefore to check (4.9) it suffices to prove that the map

$$L^2(\mathbb{R}^3, \mathrm{d}X) \ni u \mapsto \langle x\rangle^{3/2+\epsilon}\rho(x-X)\langle X\rangle^{-3/2-\epsilon}u(X) \in L^2(\mathbb{R}^3, \mathrm{d}X) \otimes L^2(\mathbb{R}^3, \mathrm{d}x)$$

is bounded, which is immediate since $\rho \in S(\mathbb{R}^3)$. This completes the proof of Thm. 4.1. □

4.5. **Existence of a ground state for non confined Hamiltonians.** In this subsection we state the results on existence of a ground state if the electronic potential is not confining. As explained in the beginning of this section, one has to assume a *stability condition*, meaning that states near the bottom of the spectrum of H are confined in electronic variables from energy conservation arguments.

Definition 4.10. *Let H be a Nelson Hamiltonian satisfying (E1), (B1). We assume for simplicity that the electronic potential $W(X)$ is bounded. Set for $R \geq 1$:*

$$D_R = \{u \in \mathrm{Dom} H \ | \mathbb{1}_{\{|X| \leq R\}}u = 0\}.$$

The ionization threshold *of H is*

$$\Sigma(H) := \lim_{R\to+\infty} \inf_{u \in D_R,\ \|u\|=1} (u|Hu).$$

The following theorem can easily be obtained by adapting the arguments in this section.

Theorem 4.11. *Assume hypotheses (E1), (B1), $W \in L^\infty(\mathbb{R}^3)$ and $m(x) \geq a\langle x\rangle^{-1}$ for some $a > 0$. Then if the following* stability condition *is satisfied:*

$$\Sigma(H) > \inf \sigma(H),$$

H has a ground state.

Sketch of proof. Assuming the stability condition one can prove using Agmon-type estimates as in [Gr] (see [P] for the case of the Nelson model) that if $\chi \in C_0^\infty(]-\infty, \Sigma(H)[$ then $\mathrm{e}^{\beta|X|}\chi(H_\sigma)$ is bounded uniformly in $0 < \sigma \leq \sigma_0$ for σ_0 small enough. From this fact one deduces by the usual argument that H_σ has a ground state ψ_σ and that

$$\sup_{\sigma>0} \|\langle X\rangle^N \psi_\sigma\| < \infty. \tag{4.13}$$

One can then follow the proof in [P, Thm. 1.2]. The key infrared regularity property replacing (4.9) is now

$$\sup_{\sigma>0} \|\omega^{-1} v \psi_\sigma\|_{\mathcal{H}\otimes\mathfrak{h}} < \infty.$$

This estimate follows as in the proof of (4.9) from Thm. A.8 and the bound (4.13). The details are left to the reader. □

Appendix A. Lower bounds for second order differential operators

In this section we prove various lower bounds for second order differential operators. These bounds are the key ingredient in the proof of the existence of a ground state for the Nelson model.

A.1. Second order differential operators.

Let us introduce the class of second order differential operators that will be studied in this section. Let:

$$\begin{aligned} h_0 = & \textstyle\sum_{1\leq j,k\leq d} c(x)^{-1} D_j a^{jk}(x) D_k c(x)^{-1}, \\ h = & \; h_0 + v(x), \end{aligned}$$

with a^{jk}, c, v real functions and:

$$\begin{aligned} & C_0 \mathbb{1} \leq [a^{jk}(x)] \leq C_1 \mathbb{1}, \; C_0 \leq c(x) \leq C_1, \; C_0 > 0, \\ & \partial_x^\alpha a^{jk}(x) \in O(\langle x\rangle^{-1}), \; |\alpha| \leq 1, \; \partial_x^\alpha c(x) \in O(1), \; |\alpha| \leq 2, \end{aligned} \tag{A.1}$$

$$v \in L^\infty(\mathbb{R}^d), \; v \geq 0. \tag{A.2}$$

Clearly h_0 and h are selfadjoint and positive with domain $H^2(\mathbb{R}^d)$. We will always assume that $d \geq 3$.

A.2. Upper bounds on heat kernels.

If K is a bounded operator on $L^2(\mathbb{R}^d, c^2\mathrm{d}x)$ we will denote by $K(x,y) \in \mathcal{D}'(\mathbb{R}^{2d})$ its distribution kernel. In this subsection we will prove the following theorem. We set:

$$\psi_\alpha(t,x) := \left(\frac{\langle x\rangle^2}{\langle x\rangle^2 + t}\right)^\alpha, \; \alpha > 0.$$

Theorem A.1. *Assume in addition to (A.1), (A.2) that:*

$$v(x) \geq a\langle x\rangle^{-2}, \; a > 0,$$

then there exists $C, c, \alpha > 0$ such that:

$$e^{-th}(x,y) \leq C\psi_\alpha(t,x)\psi_\alpha(t,y)e^{ct\Delta}(x,y), \; \forall\, t > 0, \; x, y \in \mathbb{R}^d. \tag{A.3}$$

If $c(x) \equiv 1$ or if h_0 is the Laplace-Beltrami operator for a Riemannian metric on $\mathbb{R}^d$, then Thm. A.1 is due to Zhang [Zh].

Remark A.2. *Conjugating by the unitary*

$$U: \begin{array}{rl} L^2(\mathbb{R}^d,\ \mathrm{d}x) \to & L^2(\mathbb{R}^d, c^2(x)\mathrm{d}x), \\ u \mapsto & c(x)^{-1}u, \end{array}$$

we obtain

$$\begin{array}{rl} \tilde{h}_0 := & Uh_0U^{-1} = c(x)^{-2}\sum_{1\le j,k\le d} D_j a^{jk}(x) D_k, \\ \tilde{h} := & UhU^{-1} = \tilde{h}_0 + v(x), \end{array}$$

which are selfadjoint with domain $H^2(\mathbb{R}^d)$. *Let* $\mathrm{e}^{-t\tilde{h}}(x,y)$ *for* $t>0$ *the integral kernel of* $\mathrm{e}^{-t\tilde{h}}$ *i.e. such that*

$$\mathrm{e}^{-t\tilde{h}}u(x) = \int_{\mathbb{R}^d} \mathrm{e}^{-th}(x,y)u(y)c^2(y)\mathrm{d}y,\ t>0.$$

Then since $\mathrm{e}^{-th}(x,y) = c(x)\mathrm{e}^{-t\tilde{h}}(x,y)c(y)$, *it suffices to prove Thm. A.1 for* $\mathrm{e}^{-t\tilde{h}}$.

By the above remark, we will consider the operator $\tilde{h}_0$ (resp. $\tilde{h}$) and denote it again by h_0 (resp. h). We note that they are associated with the closed quadratic forms:

$$Q_0(f) = \int_{\mathbb{R}^d} \sum_{j,k} \partial_j \overline{f} a^{jk} \partial_k f\ \mathrm{d}x, Q(f) = Q_0(f) + \int_{\mathbb{R}^d} |f|^2 c^2 v\ \mathrm{d}x,$$

with domain $H^1(\mathbb{R}^d)$.

Let us consider the semi-group $\{\mathrm{e}^{-th}\}_{t\ge 0}$ generated by h. Since $\mathrm{Dom}Q_0 = H^1(\mathbb{R}^d)$, we can apply [D, Thms. 1.3.2, 1.3.3] to obtain that e^{-th} is positivity preserving and extends as a semi-group of contractions on $L^p(\mathbb{R}^d, c^2\mathrm{d}x)$ for $1\le d\le\infty$, strongly continuous on $L^p(\mathbb{R}^d, c^2\mathrm{d}x)$ if $p<\infty$. In other words $\{\mathrm{e}^{-th}\}_{t\ge 0}$ is a Markov symmetric semigroup.

We first recall two results, taken from [PE] and [D].

Lemma A.3. *Assume (A.1), (A.2). Then there exist* $c, C>0$ *such that:*

$$0 \le \mathrm{e}^{-th}(x,y) \le C\mathrm{e}^{ct\Delta}(x,y), \forall\ 0<t,\ \ x,y\in\mathbb{R}^d.$$

Proof. Since $v(x)\ge 0$ it follows from the Trotter-Kato formula that

$$0 \le \mathrm{e}^{-th}(x,y) \le \mathrm{e}^{-th_0}(x,y),\ \text{a.e. } x,y.$$

The stated upper bound on $\mathrm{e}^{-th_0}(x,y)$ is shown in [PE, Thm. 3.4]. □

The following lemma is an extension of [D, Lemma 2.1.2] where the case $c(x)\equiv 1$ is considered.

Lemma A.4. *Assume (A.1), (A.2). Then:*

(1) e^{-th} *is ultracontractive, i.e.* e^{-th} *is bounded from* L^2 *to* L^∞ *for all* $t>0$, *and*

$$c_t := \|e^{-th}\|_{L^2\to L^\infty} = \sup_{f\in L^2} \frac{\|e^{-th}f\|_\infty}{\|f\|_2} \le ct^{-d/4}$$

with some constant $c>0$.

(2) e^{-th} *is bounded from* L^1 *to* L^∞ *for all* $t>0$ *and*

$$\|e^{-th}\|_{L^1\to L^\infty} \le c_{t/2}^2.$$

(3) *The kernel* $e^{-th}(x,y)$ *satisfies:*

$$0 \le e^{-th}(x,y) \le c_{t/2}^2.$$

Proof. From Lemma A.3 we obtain that

$$\|\mathrm{e}^{-th}f\|_\infty \le C\|\mathrm{e}^{ct\Delta}|f|\|_\infty \le C't^{-d/4}\|f\|_2,$$

using the explicit form of the heat kernel of the Laplacian. This proves (1).

Taking adjoints we see that e^{-th} is also bounded from L^1 to L^2 with $\|e^{-th}\|_{L^1\to L^2} \le c_t$. It follows that

$$\|\mathrm{e}^{-th}\|_{L^1\to L^\infty} \le \|\mathrm{e}^{-th/2}\|_{L^2\to L^\infty}\|\mathrm{e}^{-th/2}\|_{L^1\to L^2} \le c_{t/2}^2,$$

which proves (2). Statement (3) is shown in [D, Lemma 2.1.2]. □

We will deduce Thm. A.1 from the following result.

Theorem A.5. *Assume the hypotheses of Thm. A.1. Then there exists $C, \alpha > 0$ such that:*

$$e^{-th}(x,y) \le Ct^{-d/2}\psi_\alpha(t,x)\psi_\alpha(t,y).$$

Proof of Theorem A.1:
Combining Lemma A.3 with Thm. A.5 we get:

$$\begin{aligned}
\mathrm{e}^{-th}(x,y) = {} & \left(\mathrm{e}^{-th}(x,y)\right)^\epsilon \left(\mathrm{e}^{-th}(x,y)\right)^{1-\epsilon} \\
\le {} & Ct^{-\epsilon d/2}\mathrm{e}^{-\epsilon(x-y)^2/2t}t^{-(1-\epsilon)d/2}\psi_\alpha(t,x)^{1-\epsilon}\psi_\alpha(t,y)^{1-\epsilon} \\
\le {} & C't^{-d/2}\mathrm{e}^{-c(x-y)^2/2t}\psi_\beta(t,x)\psi_\beta(t,y),
\end{aligned}$$

for $\beta = (1-\epsilon)\alpha$. This completes the proof of Thm. A.1. □

It remains to prove Theorem A.5. To this end, we employ the following abstract result.

Lemma A.6. *(*[MS, Theorem B]*) Let $(M, d\mu)$ be a locally compact measurable space with σ-finite measure μ and let A be a non-negative self-adjoint operator on $L^2(M, d\mu)$ such that*

(i) *$e^{-tA_1} := (e^{-tA}|_{L^1\cap L^2})^{\mathrm{clos}}_{L^1\to L^1}$, $t \ge 0$ is a C_0-semi-group of bounded operators, i.e.,*

$$\|e^{-tA_1}\|_{L^1\to L^1} \le c_1, \quad t \ge 0.$$

(ii) *e^{-tA} is bounded from L^1 to L^∞ with:*

$$\|e^{-tA_1}\|_{L^1\to L^\infty} \le c_2 t^{-j}, \quad t > 0,$$

for some $j > 1$.

Assume moreover that there exists a family of weights $\psi(s,x)$ $(s > 0)$ such that:

(B1) $\psi(s,x)$, $\psi(s,x)^{-1} \in L^2_{\mathrm{loc}}(M \setminus N, d\mu)$ for all $s > 0$, where N is a closed null set.

(B2) There is a constant $\tilde{c}$ independent of s such that, for all $t \le s$,

$$\|\psi(s,\cdot)e^{-tA}\psi(s,\cdot)^{-1}f\|_1 \le \tilde{c}\|f\|_1, \quad f \in D_s,$$

where $D_s := \psi(s,\cdot)L^\infty_{\mathrm{c}}(M \setminus N, d\mu)$

(B3) There exists $0 < \epsilon < 1$ and constants $\hat{c}_i > 0$, $i = 1, 2$ such that for any $s > 0$ there exists a measurable set $\Omega^s \subset M$ with

(a) $|\psi(s,x)|^{-\epsilon} \le \hat{c}_1$ for all $x \in M \setminus \Omega^s$,

(b) $|\psi(s,x)|^{-\epsilon} \in L^q(\Omega^s)$ and $\||\psi(s,\cdot)|^{-\epsilon}\|_{L^q(\Omega^s)} \le \hat{c}_2 s^{j/q}$ with $q = 2/(1-\epsilon)$ and $j > 1$ is the exponent in condition (ii).

Then there is a constant C such that

$$|e^{-tA}(x,y)| \le Ct^{-j}|\psi(t,x)\psi(t,y)|, \ \forall\ t > 0, \ \text{a.e. } x, y \in M.$$

To verify condition (B2) of Lemma A.6, we will use the following lemma.

Lemma A.7. *([MS, Criterion 2]) Let e^{-tA} be a C_0-semi-group on $L^2(M, d\mu)$. Denote by $\langle\cdot,\cdot\rangle$ the scalar product on $L^2(M, \mathrm{d}\mu)$. Then:*

$$\|e^{-tA}f\|_{L^\infty} \leq \|f\|_{L^\infty}, \quad f \in L^2 \cap L^\infty, \quad t > 0,$$

if and only if:

$$\mathrm{Re}\langle f - f_\wedge, Af\rangle \geq 0, \quad f \in D(A), \tag{A.4}$$

where $f_\wedge = (|f| \wedge 1)\mathrm{sgn} f$ *with* $\mathrm{sgn} f(x) := f(x)/|f|(x)$ *if* $|f|(x) \neq 0$ *and* $\mathrm{sgn} f(x) = 0$ *if* $f(x) = 0$.

Proof of Thm. A.5: We will prove that there exists $\alpha > 0$ such that the hypotheses of Lemma A.6 are satisfied for $(M, \mathrm{d}\mu) = (\mathbb{R}^d, c^2(x)\ dx)$, $A = h$ and $\psi(s, x) = \psi_\alpha(s, x)$. For ease of notation we will often denote ψ_α simply by ψ.

From the discussion before Lemma A.4, we know that e^{-th} extends as a C_0-semi-group of contractions of $L^1(\mathbb{R}^d, c^2\mathrm{d}x)$, which implies that hypothesis (i) holds with $c_1 = 1$. Hypothesis (ii) with $j = d/2$ follows from (2) of Lemma A.4. Note that $d/2 > 1$ since $d \geq 3$.

We now check that conditions (B) are satisfied by ψ_α provided we choose $\alpha = \alpha_0 a^{\frac{1}{2}}$ for some constant α_0. Since $\psi,\ \psi^{-1}$ are bounded, condition (B1) is satisfied for all $\alpha > 0$. Set $\Omega^s := \{x \in \mathbb{R}^d \mid \langle x\rangle^2 \leq s\}$. Then

$$\psi(x)^{-\epsilon} = \left[\frac{\langle x\rangle^2 + s}{\langle x\rangle^2}\right]^{\alpha\epsilon} \leq 2^{\alpha\epsilon},\ \forall\ x \notin \Omega^s,$$

which proves the bound (a) of (B3) for all $\alpha > 0$. Take now $0 < \epsilon < \frac{d}{d+4\alpha}$ so that we see that $d - 2\alpha\epsilon q > 0$ for $q = 2/(1-\epsilon)$. If $0 \leq s < 1$ $\Omega^s = \emptyset$ and (b) of (B3) is satisfied. If $s \geq 1$ we have:

$$\begin{aligned}
\|\psi^{-\epsilon}\|^q_{L^q(\Omega^s)} &= \int_{\Omega^s}\left[\frac{\langle x\rangle^2 + s}{\langle x\rangle^2}\right]^{\alpha\epsilon q} c^2(x)\mathrm{d}x \\
&\leq C_1^2(2s)^{\alpha\epsilon q}\int_{\{|x|\leq\sqrt{s}\}} |x|^{-2\alpha\epsilon q}\mathrm{d}x \\
&= Cs^{\alpha\epsilon q}\int_0^{\sqrt{s}} r^{d-2\alpha\epsilon q-1}\mathrm{d}r = C's^{d/2}.
\end{aligned}$$

Hence (b) is satisfied for $j = d/2$.

It remains to check (B2). To avoid confusion, we denote by $\langle g, f\rangle$ the scalar product in $L^2(\mathbb{R}^d, c^2(x)\mathrm{d}x)$ and by $(g|f)$ the usual scalar product in $L^2(\mathbb{R}^d, \mathrm{d}x)$.

Since $\psi,\ \psi^{-1}$ are C^∞ and bounded with all derivatives, we see that $\{\psi\mathrm{e}^{-th}\psi^{-1}\}_{t\geq 0}$ is a C_0-semi-group on $L^2(\mathbb{R}^d, c^2\mathrm{d}x)$, with generator

$$h_\psi := \psi h\psi^{-1},\ \mathrm{Dom} h_\psi = H^2(\mathbb{R}^d).$$

We claim that there exists $\alpha > 0$ such that

$$\|\mathrm{e}^{-th_\psi}\|_{L^1\to L^1} \leq C,\ \text{uniformly for } 0 \leq t \leq s. \tag{A.5}$$

By duality, (A.5) will follow from (A.6):

$$\|\mathrm{e}^{-th^*_\psi}\|_{L^\infty\to L^\infty} \leq C,\ \text{uniformly for } 0 \leq t \leq s. \tag{A.6}$$

To prove (A.6), we will apply Lemma A.7. To avoid confusion, $\partial_j f(x)$ will denote a partial derivative of the function f , while $\nabla_j f(x)$ denote the product of the operator ∇_j and the operator of multiplication by the function f.

Setting $b_i = \psi^{-1}\partial_i\psi$, we have:

$$\begin{aligned} h_\psi^* = & \ \psi^{-1}h\psi \\ = & \ -c(x)^{-2}\sum_{j,k}\nabla_j a^{jk}(x)\nabla_k - \sum_{j,k}c^{-2}(x)b_j(x)a^{jk}(x)\nabla_k \\ - & \ c^{-2}(x)\nabla_j a^{jk}(x)b_k(x) + v(x) - c^{-2}(x)\sum_{j,k}b_j(x)a^{jk}(x)b_k(x) \\ = & \ -c(x)^{-2}\sum_{j,k}\nabla_j a^{jk}(x)\nabla_k - 2c(x)^{-2}\sum_{j,k}b_j(x)a^{jk}(x)\nabla_k + w(x), \end{aligned}$$

where:

$$\begin{aligned} w(x) = & \ v(x) - c(x)^{-2}\sum_{j,k}b_j(x)a^{jk}(x)b_k(x) \\ - & \ c(x)^{-2}\sum_{j,k}a^{jk}(x)\partial_j b_k(x) - c(x)^{-2}\sum_{j,k}(\partial_j a^{jk})(x)b_k(x). \end{aligned}$$

Clearly $\mathrm{Dom}h_\psi^* = H^2(\mathbb{R}^d)$. To simplify notation, we set $A(x) = [a^{jk}(x)]$, $F(x) = (b_1(x), \dots, b_d(x))$. The identity above becomes:

$$\begin{aligned} h_\psi^* = & \ -c^{-2}\nabla_x A\nabla_x - c^{-2}FA\nabla_x - c^{-2}\nabla_x AF + v - c^{-2}FAF, \\ = & \ -c^{-2}\nabla_x A\nabla_x - 2c^{-2}FA\nabla_x + w. \end{aligned} \tag{A.7}$$

We note that $b_j(x) = \alpha s x_j\langle x\rangle^{-2}(\langle x\rangle^2 + s)^{-1}$, which implies that:

$$|b_j(x)| \leq C\alpha\langle x\rangle^{-1},\ |\nabla_x b_j(x)| \leq C\alpha\langle x\rangle^{-2}, \text{for some } C > 0.$$

Since $v(x) \geq a\langle x\rangle^{-2}$, this implies using also (A.1) that:

$$v(x) - c(x)^{-2}FAF(x) \geq 0,\ w(x) \geq 0, \tag{A.8}$$

for $\alpha > 0$ small enough.

This implies that

$$\mathrm{Re}\langle f, h_\psi^* f\rangle = -(\nabla_x f|A\nabla_x f) + (f|(c^2 v - FAF)f) \geq 0, \quad \text{for } f \in H^1(\mathbb{R}^d). \tag{A.9}$$

It follows that h_ψ^* is maximal accretive, hence $\mathrm{e}^{-th_\psi^*}$ is a C_0-semi-group of contractions by the Hille-Yosida theorem.

To check condition (A.4) in Lemma A.7 we follow [MS], with some easy modifications. We write

$$f - f_\Lambda = \mathrm{sgn}f\chi,\ \chi := \mathbb{1}_{\{|f|\geq 1\}}(|f| - 1),$$

and note that if $f \in \mathrm{Dom}h_\psi^* \subset H^1(\mathbb{R}^d)$ then $|f|,\ \mathrm{sgn}f,\ \chi \in H^1(\mathbb{R}^d)$ with

$$\nabla\mathrm{sgn}f = \frac{\nabla f}{|f|} - f\frac{\nabla f}{|f|^2},\ \nabla\chi = \mathbb{1}_{\{|f|\geq 1\}}\nabla|f|,\ \nabla|f| = \frac{1}{2|f|}(\overline{f}\nabla f + f\nabla\overline{f}). \tag{A.10}$$

We have:

$$\begin{aligned} \langle f - f_\Lambda,\ h_\psi^* f\rangle = & \ (\nabla(f - f_\Lambda)|A\nabla f) - 2(F(f - f_\Lambda)|A\nabla f) + ((f - f_\Lambda)|c^2 wf) \\ =: & \ C_1(f) + C_2(f) + C_3(f). \end{aligned}$$

Using (A.10), we have:

$$\begin{aligned} C_1(f) = & \ (\nabla(f - f_\Lambda)|A\nabla f) \\ = & \ (\nabla f|\tfrac{\chi}{|f|}A\nabla f) - (\nabla|f||\overline{f}\tfrac{\chi}{|f|^2}A\nabla f) + (\nabla\chi|\tfrac{\overline{f}}{|f|}A\nabla f) \\ =: & \ B_1(f) + B_2(f) + B_3(f). \end{aligned}$$

Clearly $B_1(f)$ is real valued. Next:

$$\mathrm{Re}B_2(f) = -\frac{1}{2}(\nabla|f||\frac{\chi}{|f|^2}A(\overline{f}\nabla f + f\nabla\overline{f})) = -(\nabla|f||\frac{\chi}{|f|}A\nabla|f|), \tag{A.11}$$

using (A.10). Similarly:

$$\mathrm{Re}B_3(f) = \frac{1}{2}(\nabla\chi|\frac{1}{|f|}A(\overline{f}\nabla f + f\nabla\overline{f})) = (\nabla\chi|A\nabla\chi), \tag{A.12}$$

using again (A.10). We estimate now $\mathrm{Re}C_2(f)$. We have:

(A.13)
$$\mathrm{Re}C_2(f) = -2\mathrm{Re}(F(f-f_\Lambda)|A\nabla f) = \frac{1}{2}(\chi|\frac{F}{|f|}A(\overline{f}\nabla f + f\nabla\overline{f})) = -2(F\chi|A\nabla\chi).$$

We estimate now $\mathrm{Re}C_3(f)$. We have:

(A.14)
$$\mathrm{Re}C_3(f) = \mathrm{Re}(f-f_\Lambda|c^2wf) = \mathrm{Re}(\chi|c^2w|f|) = (\chi|c^2w|f|) = (\chi|c^2w\chi) + (\chi|c^2w).$$

Collecting (A.11) to (A.13), we obtain that:

$$\begin{array}{rl} \mathrm{Re}\langle f-f_\Lambda, h_\psi^* f\rangle = & (\nabla f|\frac{\chi}{|f|}A\nabla f) - (\nabla|f||\frac{\chi}{|f|}A\nabla|f|) \\ & +(\nabla\chi|A\nabla\chi) - 2(F\chi|A\nabla\chi) + (\chi|c^2w\chi). \\ & +(\chi|c^2w). \end{array} \tag{A.15}$$

We use now the point-wise identity:

$$\begin{array}{rl} & \nabla\overline{f}A\nabla f - \nabla|f|A\nabla|f| \\ = & \nabla\overline{f}A\nabla f - \frac{1}{4|f|^2}(\overline{f}\nabla f + f\nabla|f|)A(\overline{f}\nabla f + f\nabla|f|) \\ = & \frac{1}{4|f|^2}(2|f|^2\nabla\overline{f}A\nabla f - f^2\nabla\overline{f}A\nabla\overline{f} - \overline{f}^2\nabla fA\nabla f) \\ = & \frac{1}{|f|^2}(\mathrm{Re}f\nabla\mathrm{Im}f - \mathrm{Im}f\nabla\mathrm{Re}f)A(\mathrm{Re}f\nabla\mathrm{Im}f - \mathrm{Im}f\nabla\mathrm{Re}f) \geq 0. \end{array}$$

Hence the first line in the rhs of (A.15) is positive. Concerning the third line, we recall that (A.8) implies that $w \geq 0$ if $\alpha = \alpha_0 a$. Since $\chi \geq 0$ the third line is also positive. Therefore:

$$\begin{array}{rl} \mathrm{Re}\langle f-f_\Lambda, h_\psi^* f\rangle \geq & (\nabla\chi|A\nabla\chi) - 2(F\chi|A\nabla\chi) + (\chi|c^2w\chi) \\ = & \langle\chi, h_\psi^*\chi\rangle = \mathrm{Re}\langle\chi, h_\psi^*\chi\rangle, \end{array}$$

using (A.7) and the fact that χ is real. Using (A.9) we obtain condition (A.4). This completes the proof of Thm. A.5. □

A.3. **Lower bounds for differential operators.** We now deduce lower bounds for powers of h from the heat kernel bounds in Subsect. A.2.

Theorem A.8. *Assume hypotheses (A.1), (A.2) and*

$$v(x) \geq a\langle x\rangle^{-2}, \ a > 0.$$

Then

$$h^{-\beta} \leq C\langle x\rangle^{2\beta+\epsilon}, \forall\ 0 \leq \beta \leq d/2, \ \epsilon > 0.$$

We start by an easy consequence of Sobolev inequality.

Lemma A.9. *On $L^2(\mathbb{R}^d)$ the following inequality holds:*

$$(-\Delta)^{-\gamma} \leq C\langle x\rangle^{2\delta}, \ \forall\ 0 \leq \gamma < d/2, \ \delta > \gamma.$$

Proof. We have

$$(f|(-\Delta)^{-\gamma}f) = C\int\int\frac{\overline{f}(x)f(y)}{|x-y|^{d-2\gamma}}\mathrm{d}x\mathrm{d}y, \ \forall\ 0 < \gamma < n/2.$$

By the Sobolev inequality ([RS2, Equ. IX.19]):

$$\int\int\frac{\overline{f}(x)f(y)}{|x-y|^{d-2\gamma}}\mathrm{d}x\mathrm{d}y \leq C\|f\|_r^2,$$

for $r = 2d/(d+2\gamma)$. We write then $f = \langle x\rangle^{-\alpha}\langle x\rangle^{\alpha}f$ and use Hölder inequality to get:

$$\|f\|_r \leq \|\langle x\rangle^{-\alpha}\|_p\|\langle x\rangle^{\alpha}f\|_q, \ p^{-1} + q^{-1} = r^{-1}.$$

We choose $q = 2$, $p = d/\gamma$. The function $\langle x\rangle^{-\alpha}$ belongs to $L^{d/\gamma}$ if $\alpha > \gamma$. This implies the lemma. □

Proof of Thm. A.8.

We first recall the formula:

$$\lambda^{-1-\nu} = \frac{1}{\Gamma(\nu+1)} \int_0^{+\infty} \mathrm{e}^{-t\lambda} t^{\nu} \mathrm{d}t, \ \nu > -1. \tag{A.16}$$

In the estimates below, various quantities like $(f|h^{-\delta}f)$ appear. To avoid domain questions, it suffices to replace h by $h+m$, $m>0$, obtaining estimates uniform in m and letting $m \to 0$ at the end of the proof. We will hence prove the bounds

$$(f|(h+m)^{-\beta} f) \leq C(f|\langle x\rangle^{2\beta+\epsilon} f), \ \forall \ f \in C_0^\infty(\mathbb{R}^d), \tag{A.17}$$

uniformly in $m > 0$. Moreover we note that it suffices to prove (A.17) for $f \geq 0$. In fact it follows from (A.16) that $(h+m)^{-\beta}$ has a positive kernel. Therefore

$$(f|(h+m)^{-\beta} f) \leq (|f||(h+m)^{\beta}|f|) \leq C(|f||\langle x\rangle^{2\beta+\epsilon}|f|) = C(f|\langle x\rangle^{2\beta+\epsilon} f),$$

and (A.17) extends to all $f \in C_0^\infty(\mathbb{R}^d)$.

We will use the bound (A.3) in Thm. A.1, noting that if (A.3) holds for some $\alpha_0 > 0$ it holds also for all $0 < \alpha \leq \alpha_0$. We use the inequality

$$\left(\frac{\langle x\rangle^2}{\langle x\rangle^2 + t}\right)\left(\frac{\langle y\rangle^2}{\langle y\rangle^2 + t}\right) \leq \frac{\langle y\rangle^2}{t},$$

and get for $f \in C_0^\infty(\mathbb{R}^d)$, $f \geq 0$:

$$\begin{aligned} h^{-\beta} f(x) = & \ c\int_0^{+\infty} t^{\beta-1}\mathrm{e}^{-th} f(x)\mathrm{d}t \\ \leq & \ C\int_0^{+\infty} t^{\beta-\alpha-1}(\mathrm{e}^{ct\Delta}\langle x\rangle^{2\alpha}) f(x)\mathrm{d}t \\ = & \ C'(-\Delta)^{\beta-\alpha}\langle x\rangle^{2\alpha}) f(x), \end{aligned}$$

as long as $\beta > \alpha$, using again (A.16). Integrating this point-wise inequality, we get that

$$(f|h^{-2\beta} f) \leq C(f|\langle x\rangle^{2\alpha}(-\Delta)^{-2(\beta-\alpha)}\langle x\rangle^{2\alpha} f).$$

We can apply Lemma A.9 as long as $2(\beta - \alpha) < d/2$, and obtain

$$(f|h^{-2\beta} f) \leq C(f|\langle x\rangle^{4\beta+\epsilon} f), \ \forall \ \epsilon > 0,$$

if $\alpha < \beta < \alpha + d/4$. Since α can be taken arbitrarily close to 0, this completes the proof of the theorem. □

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